U.S. DEPARTMENT OF COMMERCE
NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION
NATIONAL WEATHER SERVICE

THE RED HERRING AFFAIR:

MODIFIED SEMI-IMPLICIT METHODS REVISITED

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OFFICE NOTE 64

1. Introduction

The semi-implicit integration method has been studied at considerable length at NMC since the summer of 1969. It was then that an effort began to examine A. Robert's suggestion that the method offered considerable potential for reducing the computation time required in primitive equation integrations. Following a successful application of the method to a barotropic model (McPherson, 1971), an extension to a simple baroclinic model was attempted.

Again, the path had been explored by Robert, who in turn was following the Russian Marchuk (1965). Robert's approach attempts to isolate those terms which principally govern gravitational oscillations, both external and internal, for implicit treatment. To the extent which his method is successful, the result is a stabilization of both the rapidly-moving external gravity mode and <u>all</u> of the allowable internal modes. Since at least some of the latter possess relatively low frequencies, comparable to the frequencies of the Rossby modes, the implicitization of all gravitational modes does not seem to be necessary.

Moreover, this approach in practice requires the solution of a boundary-value problem at each time step. This problem can be phrased as a coupled system of two-dimensional Helmholtz-type equations, one per model layer. Very early in the development of the semi-implicit extension to baroclinic models, it was realized that in a model with many layers, the solution of such a large boundary-value problem might be very time-consuming. Accordingly, an effort was initiated to examine possible modifications of the method so that only the external gravity mode and the fastest of the internal modes would be treated implicitly. It was felt that if this could be done, the size of the resulting system of Helmholtz equations could be reduced, while a relatively long time step could still be used.

The first abortive attempt was documented in Office Note 52. Subsequent experiments did not illuminate a way to separate external from internal modes in the difference equations. It was, therefore, concluded that further study would be unprofitable. An account of these experiments is given in Office Note 53, at the conclusion of which the carcass of the modified semi-implicit method was buried. Shortly, thereafter, Shuman (Office Note 54) suggested that the burial had been premature, and urged its resurrection. When the grave was opened, a red herring disguised as good idea leaped out and led us on a merry chase. This note is an account of our adventures.

2. <u>The state of the difference equations on the funereal occasion</u>

In Section 4 of Office Note 53, the linearized difference equation for a model in one horizontal dimension were given as

$$\frac{u^{n+1} - u^{n-1}}{2\Delta t} + \frac{1}{2}\left(\phi^{n+1} + \phi^{n-1}\right)_x + \frac{1}{2}\,\bar{\alpha}\,\sigma\left(p^{n+1} + p^{n-1}\right)_x = 0 \qquad \text{F-1}$$

$$\frac{p_*^{n+1} - p_*^{n-1}}{2\Delta t} + \frac{1}{2}\,\bar{p}_*\,\overline{\left(u^{n+1} + u^{n-1}\right)_x}^{\sigma} = 0 \qquad \text{F-2}$$

$$c_p\,\frac{T^{n+1} - T^{n-1}}{2\Delta t} - \bar{\alpha}\,\sigma\,\frac{p_*^{n+1} - p_*^{n-1}}{2\Delta t} + c_p\,\bar{\Gamma}\,\dot{\sigma}^n = 0 \qquad \text{F-3}$$

$$\left(\phi_\sigma^{n+1} + \phi_\sigma^{n-1}\right) + \bar{\alpha}\left(p_*^{n+1} + p_*^{n-1}\right) + \bar{p}_*\left(\alpha^{n+1} + \alpha^{n-1}\right) = 0 \qquad \text{F-4}$$

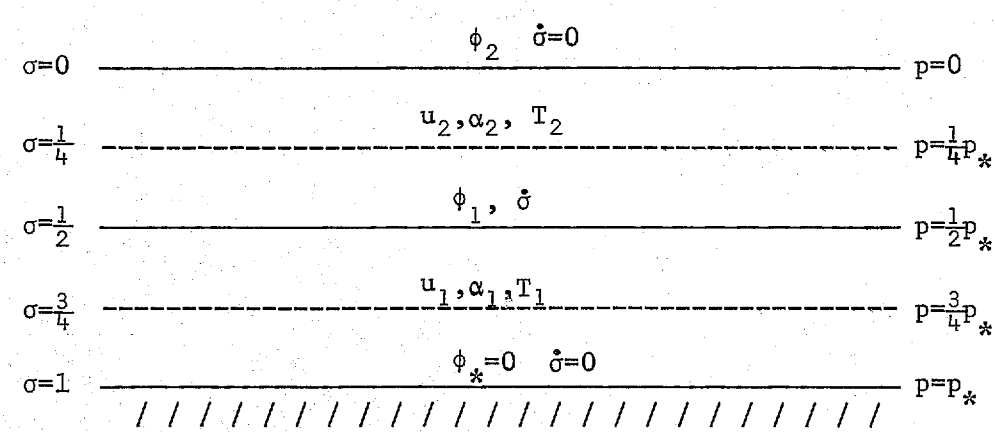
$$\sigma\,\bar{p}_*\left(\alpha^{n+1} + \alpha^{n-1}\right) + \sigma\,\bar{\alpha}\left(p_*^{n+1} + p_*^{n-1}\right) - R\left(T^{n+1} + T^{n-1}\right) = 0 \qquad \text{F-5}$$

$$\dot{\sigma}_{\sigma\sigma} = \frac{1}{2}\left(u^n\right)_{x\sigma}\ . \qquad \text{F-6}$$

These equations are based on Phillips' σ-vertical coordinate,

$$\sigma = p/p_*\ .$$

The overbar notation denotes a basic state quantity, the $(-\sigma)$ notation denotes a vertical average, and spatial differencing is indicated by a subscript (x) or (σ). The analyses discussed in Office Note 53, as well as those of subsequent sections of this note, were performed in the framework of a two-layer representation of a fluid, as illustrated below.



Such a vertical structure allows a free mode with phase speed of 306 m sec^{-1}, and one corresponding to an internal mode, with phase speed of 81 m sec^{-1}. These values were calculated on the basis of an isothermal basic state at 250 K in Office Note 47.

The computational stability analysis of the system (F-1, F-6) presented in Office Note 53 indicated that the system is stable regardless of the time step, except that the computational mode corresponding to the internal gravity wave is unstable. The reason for this was not clearly understood until Shuman analyzed it in Office Note 54. He showed that a "mixed" implicit-explicit formulation of the linear equation for a homogeneous fluid with a free surface behaved in a manner similar to that we had described. He also demonstrated that some "mixed" formulations may be stable, and gave an example of one such system which is not only stable but allows a time step twice as long as the usual leapfrog scheme. This technique has since been examined by Brown and Campana (1971), who have found it to be suitable for operational implementation.

From Shuman's work, then, came the suggestion that the mixed implicit-explicit formulation might yet be made to work, but it appeared that we would have to be siezed by an attack of craftiness to pick out a stable mixture.

3. The Sum-and-Difference Method I

Arguing that the external mode is primarily associated with the integrated divergence field, while the internal mode is primarily associated with the divergence of the vertical shear, we first replaced the two momentum equations (one per layer) by an equation for the sum of the winds and one for the difference:

$$\frac{\partial}{\partial t}\left(\frac{u_1+u_2}{2}\right) + \frac{1}{4}\frac{\partial}{\partial x}\left(2\phi_1+\phi_2\right) + \frac{1}{8}(3\overline{\alpha}_1+\overline{\alpha}_2)\frac{\partial p_*}{\partial x} = 0$$

and

$$\frac{\partial}{\partial t}\left(\frac{u_1-u_2}{\Delta\sigma}\right) - \left(\frac{1}{2\Delta\sigma}\right)\frac{\partial\phi_2}{\partial x} + \left(\frac{1}{4\Delta\sigma}\right)(3\overline{\alpha}_1-\overline{\alpha}_2)\frac{\partial p_*}{\partial x} = 0 .$$

We then treated the vertically-integrated equation implicitly, and the vertically-differentiated equation explicitly:

$$\left(\frac{u_1^{n+1}-u_1^{n-1}+u_2^{n+1}-u_2^{n-1}}{2\Delta t}\right) + \tfrac{1}{2}\left(\phi_1^{n+1}+\phi_1^{n-1}\right)_x + \tfrac{1}{4}\left(\phi_2^{n+1}+\phi_2^{n-1}\right)_x$$

$$+ \tfrac{1}{8}\left(3\overline{\alpha}_1+\overline{\alpha}_2\right)\left(p_*^{n+1}+p_*^{n-1}\right)_x = 0 \qquad \text{SI-1}$$

and

$$\frac{\left(u_1^{n+1}-u_1^{n-1}\right)-\left(u_2^{n+1}-u_2^{n-1}\right)}{2\Delta t} - \frac{1}{2}\left(\phi_2^n\right)_x + \frac{1}{4}\left(3\bar{\alpha}_1-\bar{\alpha}_2\right)\left(p_*\right)_x^n = 0 \quad . \qquad \text{SI-2}$$

The remaining equations of the set are as given in eqns. (F2-F6). The system of equations thus features an implicit treatment of the vertically-integrated wind in the momentum equation and the continuity equation (F-2), and explicit treatment of the equation for the wind shear, the diagnostic equation in $\dot{\sigma}$ (F-6), and the stability term in the thermodynamic equation (F-3).

We then substituted a trial solution of the form $Q = Q_o \zeta^n e^{ikx}$, as in previous analyses, and eventually arrived at a pair of equations in ζ, the time-dependent part of the solution:

$$\left\{(\zeta^2-1)^2 + \frac{1}{8}\,\varepsilon^2(\zeta^2+1)^2\ (\kappa+1)(3\bar{\alpha}_1+\bar{\alpha}_2)\bar{p}_*\right\}p_* - \left\{\varepsilon^2\Delta t\ \bar{p}_* R\bar{\Gamma}\ \frac{\zeta(\zeta^2+1)^2}{(\zeta^2-1)}\right\}\dot{\sigma} = 0$$

and

$$\left\{\frac{1}{8}\,k\ \varepsilon\ [\bar{\alpha}_1(\kappa-3) + \bar{\alpha}_2(\kappa+1)][\zeta(\zeta^2-1)]\right\}p_* + \left\{(\zeta^2-1)^2 - \frac{2}{3}\,\varepsilon^2\ R\bar{\Gamma}\ \zeta^2\right\}\dot{\sigma} = 0\ ,$$

where $\varepsilon = k\Delta t$, $\kappa = R/c_p$, and the subscripts 1 and 2 refer to the lower and upper layers of the model respectively. If nontrivial solutions exist, the determinant of these two equations must vanish. This requirement leads to an eighth-order polynomial in ζ the roots of which must be evaluated numerically for a given basic state. The procedure followed was as outlined in Office Note 52. We defined

$$\varepsilon_m = m\ k\Delta t = \frac{2\pi m}{3.81}\ .\ 10^{-5}(\text{cm}^{-1}\text{sec})$$

and then evaluated the determinant of the above equations for $m=1,2,\ldots 7$, (and an isothermal basic state at 250 k) over the complex plane. For each m, the loci of the zeros of the determinant, corresponding to the roots of the polynomial, were calculated. For stability, no root should be located outside the unit circle of the complex plane. Neutral response is indicated by roots on the unit circle, and damping by roots inside the unit circle.

The results of this procedure are shown in Figure 1. Roots corresponding to the external mode (identified by the greater phase angle) lie on the unit circle until $m = 5$, but are outside for larger values. For comparison, the analogous roots in explicit leapfrog scheme remain on the unit circle only up to $m \simeq 2$. Thus, this method does not completely stabilize the external mode, but does relax somewhat the stability criterion associated with it. In principle, if one could employ a ten-minute time step with an explicit integration method, this modified implicit method would permit a

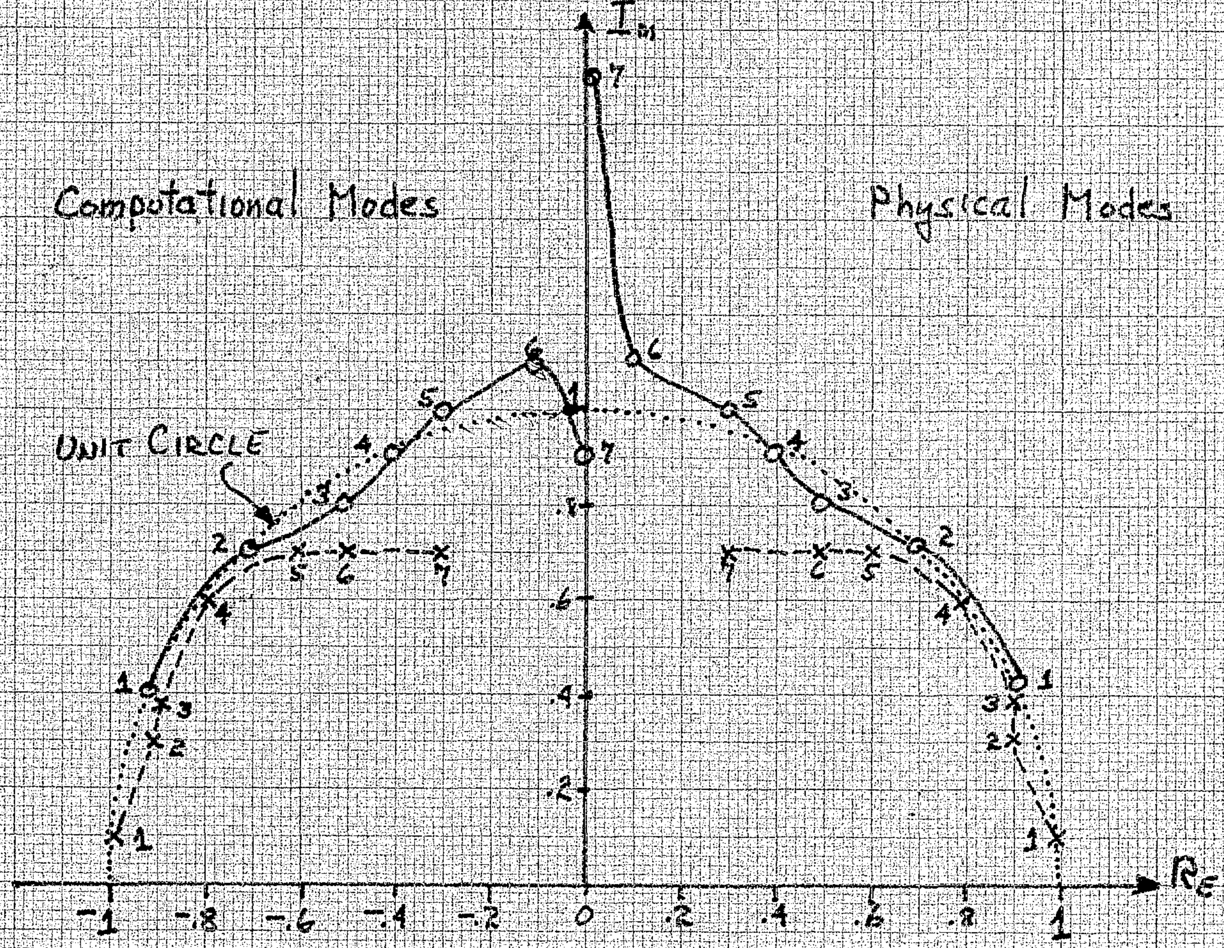


FIGURE 1. LOCI OF THE ROOTS OF THE FREQUENCY EQUATION FOR SUM-AND-DIFFERENCE METHOD I. THE EXTERNAL MODE IS REPRESENTED BY THE SOLID TRACE AND THE INTERNAL MODE BY THE DASHED TRACE. THE NUMBERS BESIDE EACH ROOT INDICATE THE VALUE OF m.

25 minute time step. Only one Helmholtz-type equation, in the surface pressure p_*, would have to be solved at each time step.

However, the stable "mixed" scheme proposed by Shuman and employed by Brown and Campana would allow a 20 minute time step, with no boundary value problem to solve. This sum-and-difference method therefore appeared to be of little economic value. Moreover, the fact that it is the external mode which becomes unstable first indicated that our objective had not achieved.

4. The Resurrection Method I

The discouraging results of the experiment described in the preceding section led us to cast about for another approach. After considerable experimentation, we arrived at the idea of formally replacing the geopotentials in the momentum equations through the use of the hydrostatic equation:

$$\frac{\partial u_1}{\partial t} + \overline{\alpha}_1 \frac{\partial p_*}{\partial x} + \frac{1}{4}\,\overline{p}_* \frac{\partial \alpha_1}{\partial x} \,,$$

and

$$\frac{\partial u_2}{\partial t} + \frac{1}{2}(\overline{\alpha}_1+\overline{\alpha}_2)\frac{\partial p_*}{\partial x} + \frac{1}{4}\,\overline{p}_* \frac{\partial}{\partial x}(2\alpha_1 + \alpha_2) = 0$$

We then argued that we could possibly effect the desired separation of external and internal modes by treating the pressure-gradient terms implicitly and the specific-volume-gradient terms explicitly. Thus, eqns. (SI-1, SI-2) were replaced by

$$\frac{u_1^{n+1} - u_1^{n-1}}{2\Delta t} + \frac{1}{2}\,\overline{\alpha}_1\left(p_*^{n+1} + p_*^{n-1}\right)_x + \frac{1}{4}\,\overline{p}_*(\alpha_1)_x^n = 0 \qquad \text{RI-1}$$

and

$$\frac{u_2^{n+1} - u_2^{n-1}}{2\Delta t} + \frac{1}{4}(\overline{\alpha}_1 + \overline{\alpha}_2)\left(p_*^{n+1} + p_*^{n-1}\right)_x + \frac{1}{4}\,\overline{p}_*(2\alpha_1^n + \alpha_2^n)_x = 0 \qquad \text{RI-2}$$

but the rest of the equations remained unaltered.

A similar evaluation of the roots of the frequency equation was performed, again for an isothermal basic state at 250 K. The loci of the roots are plotted in Figure 2 for $m=1,2,\ldots,7$. As in the previous case, the external mode becomes unstable first, but for an even smaller value of m. According to the results of this analysis, the method in question would permit a time step of only twice that permitted by an explicit scheme, and a boundary-value problem would still have to be solved at each time step. Clearly, this was an unacceptable result.

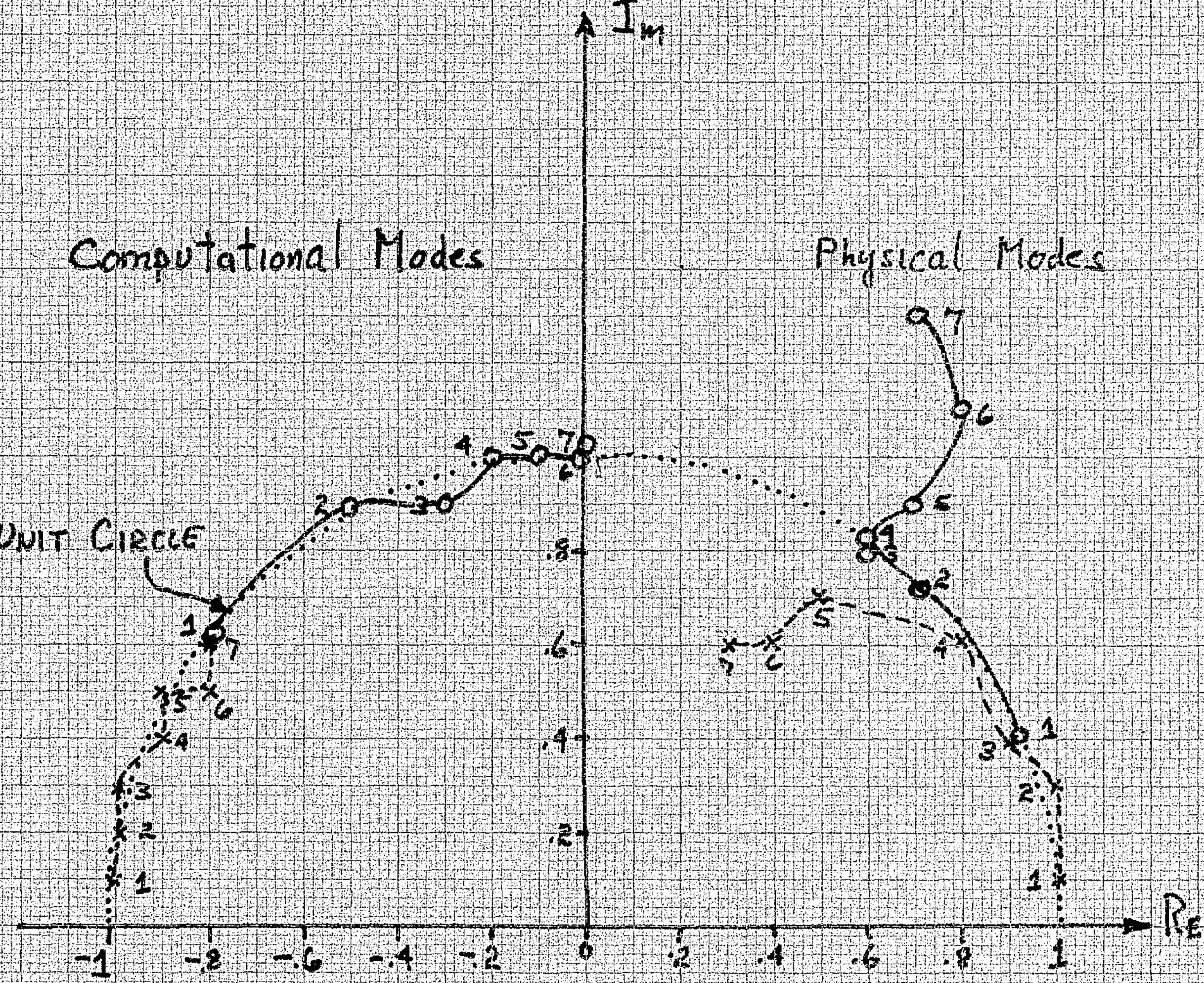


FIGURE 2. SAME AS FIGURE 1, BUT FOR THE RESURRECTION METHOD I.

5. The Sum-and-Difference Method II

One of the ideas to emerge following Shuman's discussion of "mixed" systems is that one can arrange a mixture such that the result is precisely equivalent to an explicit leapfrog scheme. Consider the linear equations governing a homogeneous fluid with a free surface,

$$\frac{\partial u}{\partial t} + g\,\frac{\partial h}{\partial x} = 0$$

$$\frac{\partial h}{\partial t} + H\,\frac{\partial u}{\partial x} = 0\ ,$$

where h is the depth of the fluid, and H is its mean depth. Using centered time differences, one can write the analogous difference equations as

$$\frac{u^{n+1} - u^{n-1}}{2\Delta t} + ik\,g\,h^{n+1} = 0$$

$$\frac{h^{n+1} - h^{n-1}}{2\Delta t} + ik\,H\,u^{n-1} = 0\ ,$$

where trigonometric spatial dependence ($u,\ h \sim e^{ikx}$) has been assumed. Note that the height gradient term in the momentum equation is evaluated at time $t = (n+1)\Delta t$, which has been called a "backward" implicit approximation by Kurihara (1965). The divergence term in the continuity equation is evaluated at $t = (n-1)\Delta t$, which is a "forward" scheme. By itself, the "backward" approximation can be demonstrated to be damping, while it is well known that the "forward" scheme is amplifying. It is easy to show that their combination is equivalent to the customary leapfrog method.

Assume that $u,\ h \sim \zeta^n$, so that the equations become

$$(\zeta^2-1)u + (2ik\Delta tg\zeta^2)h = 0$$

$$(2ik\ tH)u + (\zeta^2-1)h = 0$$

The determinant of this system must vanish, which leads to the frequency equation

$$\zeta^2 \pm (2ikc\Delta t)\zeta - 1 = 0,$$

where $c = \sqrt{gH}$. This is identically the frequency equation associated with the leapfrog scheme.

It seemed that this idea might be employed in the problem of separation of the external and internal modes. In the first Sum-and-Difference method, we had evaluated both the shear-momentum equation (SI-2) and the thermodynamic equations explicitly. This formulation failed to stabilize the external mode, although the vertically-integrated equation of motion and the continuity equation were treated implicitly. We were led to suspect, then, that the shear momentum equation must contain some influence on the external mode, so that an explicit evaluation would not be adequate. At this point, we postulated that if this equation were evaluated by a "backward" implicit approximation, the result would stabilize (and possibly damp) the external mode, to the extent that the shear-momentum equation governs the external mode. But to the extent that the equation governs the internal mode, we argued that the "backward" evaluation should be combined with a "forward" evaluation of the stability term of the thermodynamic equation. In this way, it was expected that the internal mode would effectively be evaluated explicitly.

The vertically-differenced equation (SI-2) was thus replaced by

$$\frac{(u_1^{n+1}-u_1^{n-1}) - (u_2^{n+1}-u_2^{n-1})}{2\Delta t} - \frac{1}{2}(\phi_2)_x^{n+1} + \frac{1}{4}(3\bar{\alpha}_1-\bar{\alpha}_2)(p_*)_x^{n+1} = 0 \qquad \text{SII-2}$$

and the thermodynamic equation was modified to employ a "forward" evaluation of the stability term:

$$c_p\frac{T^{n+1}-T^{n-1}}{2\Delta t} - \bar{\alpha}\,\sigma\frac{p_*^{n+1}-p_*^{n-1}}{2\Delta t} + c_p\bar{\Gamma}\,\dot{\sigma}^{n-1} = 0 \ . \qquad \text{SII-3}$$

The results of the computational stability analysis of this system are plotted in Figure 3. The internal mode is seen to be treated neutrally; i.e., all roots lie on the unit circle for the range of values of m. But again, the external mode becomes unstable, although at a value of m slightly in excess of 6. This represents a further relaxation of the stability criterion associated with the external mode...a 30-minute time step would be allowed if an explicit method permitted a 10-minute time step...but the objective of stable treatment, regardless of time step, of the external mode, remained out of reach.

6. The Resurrection Method II

We next decided that, because of the damping properties of the "backward" approximation, we could evaluate all of the terms of the momentum equations at time $t = (n+1)\Delta t$, while retaining the "forward" approximation of the stability term in the thermodynamic equation. In this way, we anticipated that the external mode would be stable, and damped, for any time step, while the internal mode would be calculated

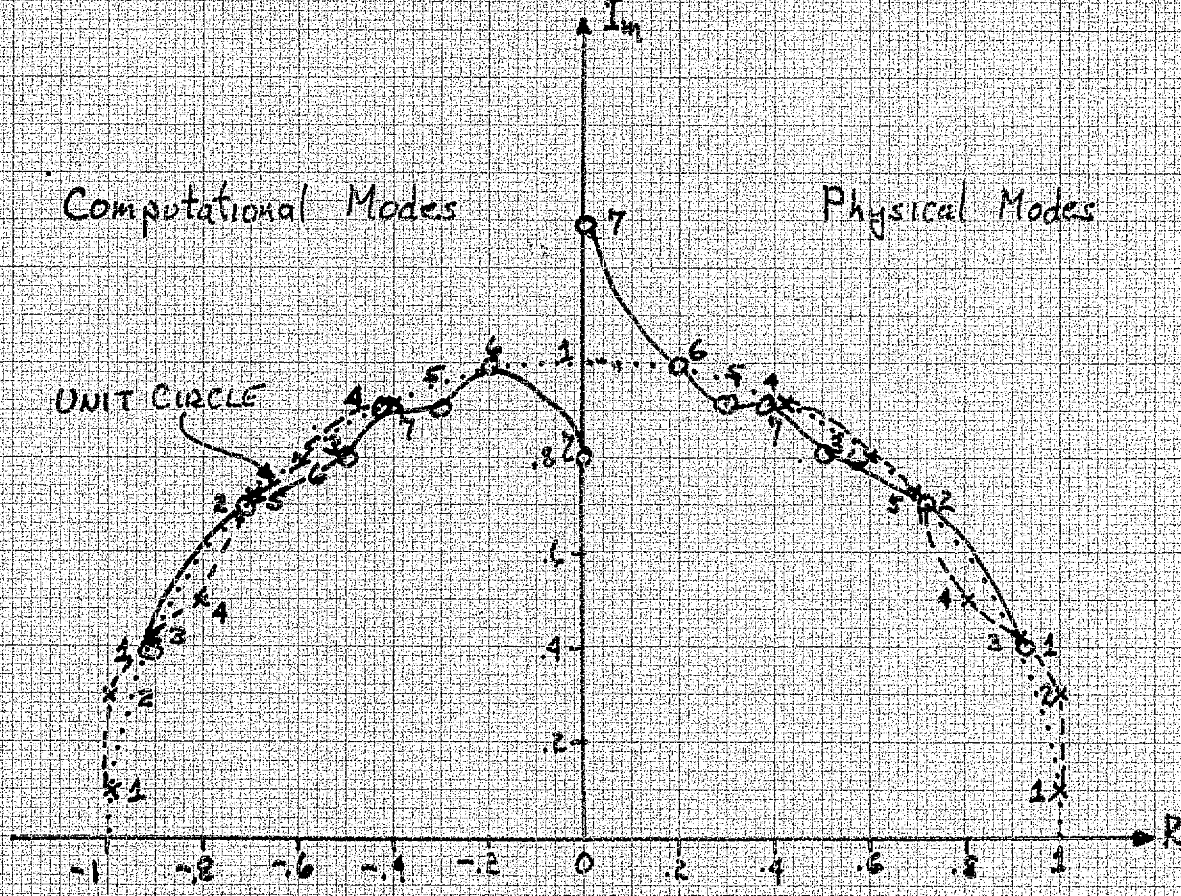


FIGURE 3. SAME AS FIGURE 1, BUT FOR THE SUM-AND-DIFFERENCE METHOD II.

explicitly as in the previous experiment. It was decided to try this without the sum-and-difference formulation, since that system is somewhat awkward to use. Thus the momentum equations corresponding to (RI-1, RI-2) were rewritten as

$$\frac{u_1^{n+1}-u_1^{n-1}}{2\Delta t} + \overline{\alpha}_1 (p_*)_x^{n+1} + \frac{1}{4}\,\overline{p}_* (\alpha_1)_x^{n+1} = 0 \qquad \text{RII-1}$$

$$\frac{u_2^{n+1}-u_2^{n-1}}{2\Delta t} + \frac{1}{2}(\overline{\alpha}_1+\overline{\alpha}_2)(p_*)_x^{n+1} + \frac{1}{4}\,\overline{p}_* (2\alpha_1^{n+1}+\alpha_2^{n+1})_x = 0 \qquad \text{RII-2}$$

The thermodynamic equation was retained in the form (SII-2), and, for consistency, the continuity equation (F-2) was rewritten as

$$\frac{p_*^{n+1}-p_*^{n-1}}{2\Delta t} + \frac{1}{2}\,\overline{p}_* (u_1^{n+1}+u_2^{n+1})_x = 0\ . \qquad \text{RII-3}$$

The remaining equations, the ideal gas law and the diagnostic equation in $\dot{\sigma}$, were unchanged.

Figure 4 displays the results of the computational stability analysis. As anticipated, the external mode is strongly damped as the parameter m increases. The internal mode is calculated explicitly, and becomes unstable when m is sufficiently large to violate the ordinary linear stability criterion for a wave with a phase speed of 81 m sec^{-1}.

With this result, the objective of separating the external and internal modes had been achieved. In order to confirm the results of these analyses, experimental integrations were performed with two-layer models based on the differencing systems discussed in Sections 4, 5, and 6, together with a completely explicit and a completely implicit formulation. These integrations were performed in one horizontal dimension, with a staggered grid such that the winds u_1, u_2 were defined as points midway between points where the thermodynamic variables were defined. The mesh length (distance between adjacent values of the same quantity) was 762 km, the basic state was assumed isothermal at 250 K, and $\overline{p}_*$= 1000 mb. The winds were initially given by

$$u = 10 \sin\left(\frac{2\pi x.10}{L}\right) \qquad \text{(wave \#10)}$$

where L = 49Δx, and cyclic continuity was prescribed on the lateral boundaries. The results of these integrations are summarized in the following table.

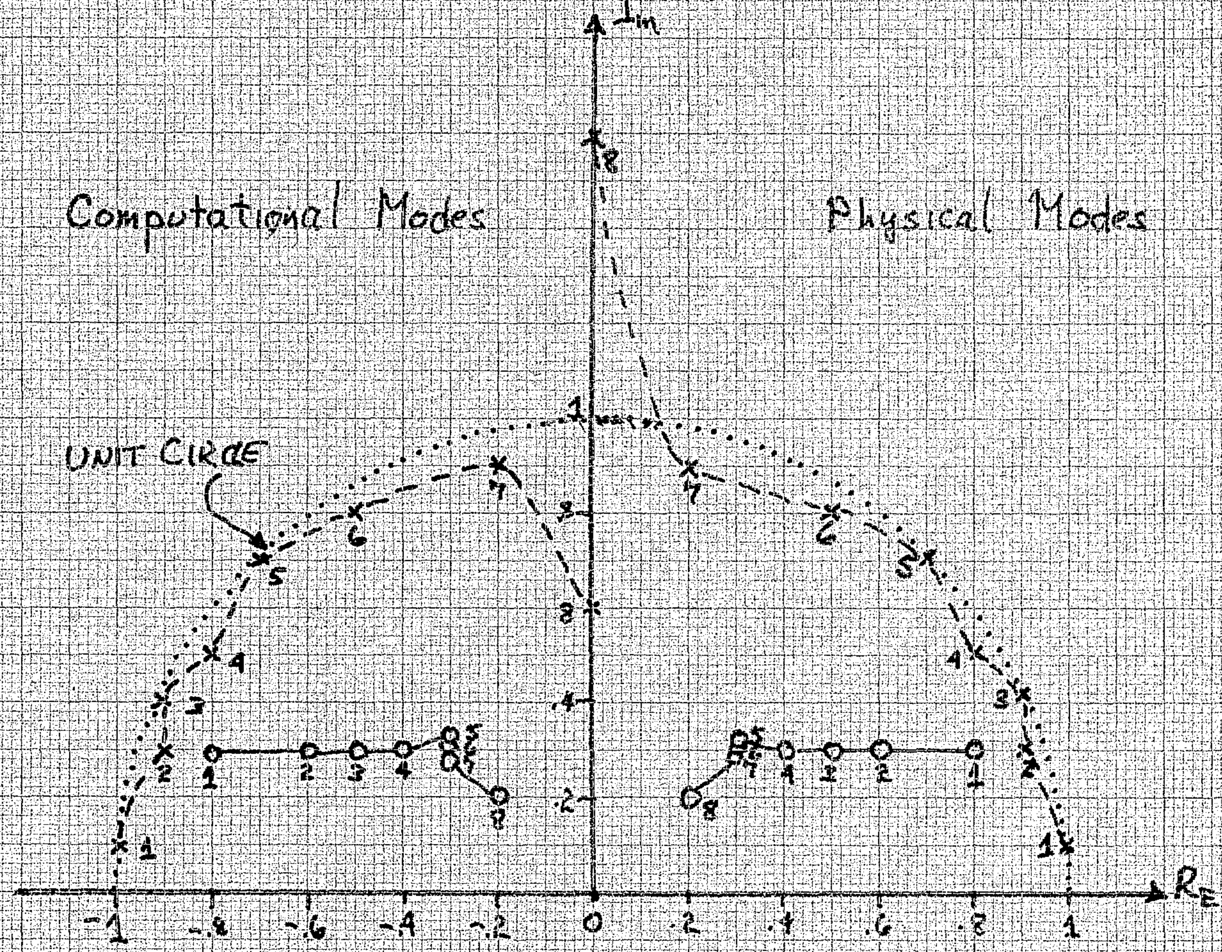


FIGURE 4. SAME AS FIGURE 1, BUT FOR RESURRECTION METHOD II.

Method	Response	Max. Δt (minutes)	$\left(\frac{\Delta t \text{ max.}}{\Delta t \text{ explicit}}\right)_{\text{numerical}}$	$\left(\frac{\Delta t \text{ max.}}{\Delta t \text{ explicit}}\right)_{\text{analytic}}$
Explicit	Neutral	20	1	1
Resurrection I	Neutral	60	3	2.1
Sum-and-Diff. II	Neutral	70	3.5	3.1
Resurrection II	Damping (Ext. mode) Neutral (Int. mode)	90	4.5	3.9
Implicit	Neutral	120*	6	∞

*Longest time step tried.

The ratio $\Delta t(\max)/\Delta t(\text{explicit})$ shows some discrepancies between the evaluation from the computational stability analyses and the estimate obtained from numerical integrations. This is undoubtedly due to spatial truncation in the numerical integrations retarding the actual phase speeds of the gravitational modes. Overall, there is good agreement between theory and experiment.

7. Conclusion

With the Resurrection II scheme, we indeed have demonstrated that the external mode can be separated from the internal mode in a two-layer model, and that the former can be treated implicitly and damped, while the latter is treated explicitly with neutral response. Such a scheme has several desirable properties, among them the selective damping of the external mode, but principally that it allows a time step approximately four times that permitted by an explicit model. Only one relatively simple boundary-value problem need be solved at each time step. These results have been confirmed by limited numerical integration of a two-layer model.

Howevever, it has been suggested by W. L. Jones[1] of NCAR that the numerical phase speed of the internal gravity mode is affected by the vertical resolution in models in much the same way as horizontal resolution affects the translation of short meteorological waves. That is, the greater the resolution, the more closely the numerical phase speed approaches the analytic. This means that as the number of layers in a model increases, the numerical phase speed of the first (most rapidly-propagating) internal mode will approach a value in the range of 100-150 m sec^{-1}. If the Resurrection II method were applied to a model with many layers, the ratio of $\Delta t(\max)/\Delta t(\text{explicit})$ would drop to between two and three. Allowing for the time required to solve a Helmholtz-type equation each time step, the potential economy is not appreciably greater than is offered by the method Brown and Campana are studying.

To confirm this, a linear computational stability analysis of an isothermal four-layer model using Phillips' σ-coordinate and the Resurrection II method has been carried out. The model is as described in Office Note 47. In that note, the phase speed of the first internal mode is calculated to be 110 m sec^{-1}. As anticipated, the analysis showed that the ratio $\Delta t(\max)/\Delta t(\text{explicit})$ would be approximately three.

It therefore appears that the application of the Resurrection II method to a multilevel model is not justifiable solely on economic grounds. However, one might consider employing it to take advantage of its other properties; for example, the selective damping of the external mode. At the present time, it seems more profitable to adopt the unmodified semi-implicit method for use in multilayer models. We have made that decision, and do not propose to pursue the red herring any further.

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[1] Personal communication

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